SESSION A25 DMP:
THEORY OF MATERIALS I:
LARGE-SCALE APPROACHES
Monday morning, 20 March 1995
Regency Ballroom I, Fairmont Hotel, at 8:00
N. Trouiller. presiding

'Invited paper

8:00

A251 **Electronic** Structure **of 1000 Atom Semiconductor Quamtum Structures via Pseudopotential Calcula-**

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We have developed an approach which uses screened pseudopotentials and a plane wave basis to calculate the electronic structure for semiconductor thousand atom nanoscale quantum systems. A screened spherical pseudopotential is first fitted to a few first principle bulk total potentials, then is modifed to fit the experimental band structure. This produces a pseudopotential which is accurate for its wavefunctions and band energies, and is transferable to different crystal structures and unit cell volumes. Using such pseudopotentials, we can construct nonselfconsistently the total potential of a large system. To find the electronic structure **for such a** system for the given potential, we have developed three methods: (1) the "folded spectrum" method' [1] which finds the band edge states (e.g, the valence band maximum and conduction band minimum) without calculating all states below them and which scales linearly with the number of atom Nat *(2)* the "generalized moments" methods which calculates the density of states and optical absorption spectrum, and whose computing time is roughly independent of Nat (3) the Lanczos method[3] which can calculate all occupied states and scales roughly as the square of Nat These methods are much faster than the widely used preconditioning conjugate gradient method, making possible calculations for thousand atom systems in one or two Cray-90 YMP CPU hours. The current approach has been used in the study of Si quantum dots' with a local pseudopotential and CdSe quantum dots with nonlocal pseudopotentials and spin-orbit coupling. The band gap, radiative lifetime, density of states and dielectric constants are studied as functions of quantum dot size and shape. This relatively sophisticated calculation has been used to judge the accuracy of other simpler calculations and models.

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'L.W. Wang and A. Zunger, J. Chem. Phys. 100, 2394 (1994).
2L.W. Wang, Phys. Rev. B 49, 10154 (1994).
3L.W. Wang and A. Zunger, Comp. Mat. Sci. 2,326 (1994).
4L.W. Wang and A. Zunger, J. Phys. Chem. 98,2158 (1994); Phys. Rev. Lett. 73, 1039 (1994).